

Carbamic acid, ethyl-, methyl ester
6135-31-5 | DTXSID80210261

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 14.3 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.53e-01

Confidence level: 6.05e-01

Nearest Neighbors from the Training Set

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1,2-Diethylhydrazine

Measured: 15.1

Predicted: 14.1

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3-Pyridinecarbonitrile

Measured: 36.3

Predicted: 25.0

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1-Methoxy-2-propyl acetate

Measured: 2.29

Predicted: 7.33

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1,4-Dioxane

Measured: 17.0

Predicted: 13.2

Image not found

Benzamide

Measured: 28.8

Predicted: 29.7